STRUCTURAL FEATURES OF AROMATIC HYDROCARBONS CLUSTERS IN A WIDE RANGE OF STATE PARAMETERS

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The cluster formations in liquids define structural features and thermophysic properties of liquids. Earlier the authors proposed the relation for clusters distribution function in liquid on number of the particles contained in cluster [1]: $f(Z) = \frac{\lambda^m}{6} \cdot Z^{m-1} \cdot e^{-\lambda Z}, \quad Z \geq 0$, where Z is the number of particles in cluster, $\lambda > 0 \quad (\lambda = 1/\theta)$ is the scale parameter determined by physical properties of the liquid, $m = 4$ is the distribution order.

The parameter θ is the function of the molecular packing factor η: $\theta = a_1\eta + a_2\eta^2 + \ ... \ + a_n\eta^n \approx (5/2)\eta e^{\eta} \approx (5/2)(1+\eta)$, where a_i is the serial power expansion coefficients; $\eta \approx 0.22\rho^*$, where $\rho^* = \rho/\rho_c$ is the reduced density of a liquid.

Using the cluster size probability distribution on a number of particles and experimental data on the density of liquids, we have estimated and analyzed the most probable number of particles in cluster: $\hat{Z} = \frac{m-1}{\lambda} = (m-1)\theta = 3\theta$, the average number of particles in clusters: $\overline{Z} = \int_0^\infty Z \cdot f(Z)dZ = \frac{m!}{(m-1)!}\frac{1}{\lambda} = \frac{m}{\lambda} = m\theta = 4\theta$ and the root-mean-square number of particles in clusters: $\overline{\overline{Z}} = \sqrt{\bar{Z}^2} = \frac{\sqrt{m(m+1)}}{\lambda} = \sqrt{m(m+1)} \cdot \theta = \sqrt{20} \cdot \theta$ of benzene, toluene and their halogen-substituted depending on the state parameters at temperatures 293–423 K and pressures 0.1–600 MPa.

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1. Verveyko V.N., Verveyko M.V., Melnikov G.A. // Eur. Phys. J. D. 2016. V. 70. P. 47.